

The Dynamics of a Neutrally Buoyant Particle in Laminar Flow: Theory and Numerical Evaluation

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Abstract

In 1961, Segre and Silberberg discovered an interesting phenomenon, neutrally buoyant particles in Hagen-Poiseuille flow tend to focus at specific radial positions within the fluid. Subsequent studies focused on theoretical and experimental explanations of the phenomenon. The focusing effect has found its way in industrial and biochemical applications for the purpose of particle separation at high throughput. In this study, we present a framework through which the dynamical interaction between a neutrally buoyant particle and fluid can be numerically evaluated.

Keywords: Segre-Silberberg effect, Hagen-Poiseuille flow, particle separation, Computational Fluid Dynamics, CFD, biomedical application

1 Introduction

The discovery made by Segre and Silberberg [1] promoted decades of research on the mechanism [2] [3] of the tubular pinch effect where small neutrally buoyant particles form annular rings in a circular tube. It became slowly understood that the migration of the particles is caused by inertial forces acting on the particles [4] in the proximity of the walls [5]. Lateral migration of particles will occur whenever there are lateral gradients of normal stress in the undisturbed velocity field [2] [6]. Analytical models using perturbation calculation capture most essential features of the tubular pinch effect at small Reynolds numbers [3] [7] [8] [9]. The effect is also numerically validated using the Lattice Boltzmann Method for Reynolds numbers up to 1000 [10] [11] [12]. The tubular pinch effect can be applied in industrial, pharmaceutical, and biochemical particle separation devices to significantly improve throughput because the mechanism relies on fundamental fluid dynamics principles [13] [14] [15] [16].

The tubular pinch effect is relatively simple to verify through an experimental approach to some extent but it's limited by the physical constraints of the apparatus used to check the presence of the effect under more complex conditions [3] [8]. A computational fluid dynamics approach could provide a more rapid way to examine the effect under various physical conditions involving Reynolds number, tube radius, particle size, particle shape, etc. In this work, we present a complete framework based on the Navier-Stokes equations to gain more complete insight on how the particles interact with the fluid dynamically. Most Computational Fluid Dynamics (CFD) packages including OpenFOAM [17] do not have a solver that allows particle tracking, that is to dynamically update the state of the fluid and particle as the particles travel in the fluid with both translational and rotational motion. Conventional approaches in CFD packages handle particle tracking by first calculating the flow fields without the particle, then applying the flow fields on the particle. As such it misses the important aspect of the presence of the particles' effect on the flow fields. This conventional approach is done because keeping track of the particle position and its translational and rotational motion requires constant updates to the computational mesh used in the simulation. This can be computationally expensive for a large number of particles [18] [19] [20]. We present a framework in which the complete dynamical interaction between fluid and particles can be analyzed and evaluated numerically in an efficient manner.

2 Dynamics of the Interaction

We start with the Navier-Stokes equations governing the motion of a viscous, incompressible fluid.

$$\vec{\nabla} \cdot \vec{v} = 0 \quad (1)$$

$$\rho \left(\frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \vec{\nabla} \vec{v} \right) = -\vec{\nabla} p + \mu \vec{\nabla} \cdot \overleftrightarrow{\tau} + \rho \vec{f} \quad (2)$$

where the body force $\vec{f}$ is neglected in typical applications of the tubular pinch effect.

Next we include the interaction between the particle and the fluid through pressure p and the velocity stress tensor $\overleftrightarrow{\tau}$ in the unified stress tensor $\overleftrightarrow{\sigma} = -p \overleftrightarrow{I} + \mu \overleftrightarrow{\tau}$, where $\overleftrightarrow{I}$ is the identity matrix and μ is the dynamic viscosity of the fluid.

$$m \frac{d\vec{u}_{cm}}{dt} = - \oint \overleftrightarrow{\sigma} \cdot \hat{n} dA \quad (3)$$

$$\overleftrightarrow{I}_{cm} \cdot \vec{\alpha} = - \oint \vec{r} \times (\overleftrightarrow{\sigma} \cdot \hat{n}) dA \quad (4)$$

where $\vec{u}_{cm}$, $\hat{n}$, and $\vec{\alpha}$ are the translational velocity, unit normal vector, and angular acceleration of the particle. Note that from Newton's 3rd Law, the force and torque acting on the particle affect both the motion of the particle and the fluid.

The no slip boundary condition at the surface of the particle is described by

$$\hat{n} \times (\vec{v} - (\vec{u}_{cm} + \vec{\omega} \times \vec{r})) = 0 \quad (5)$$

where $\vec{\omega}$ and $\vec{r}$ are the angular velocity and center of mass position of the particle.

3 Verification

Two separate verifications are performed using the governing equations. In the first case, a uniform cube is placed in a parabolic velocity profile and the lift and torque are computed both analytically and numerically. In the second case, a uniform sphere is placed in a parabolic velocity profile and the lift and torque are computed both analytically and numerically. The results from the analytical and numerical calculations are then compared for agreement.

3.1 Initial Condition and Boundary Condition

A time independent parabolic velocity profile $v(y) = ay^2$ is applied in a computational domain bound by $0 \leq x \leq 1, 0 \leq y \leq 1$. The velocity profile also serves as the initial condition of the fluid flow. A Dirichlet boundary condition for the velocity is applied at $x = 0$ and $x = 1$, identical to the parabolic velocity profile $v(y) = ay^2$; a Neumann boundary condition for the velocity is applied at $y = 0$ and $y = 1$. A no slip boundary condition is applied at the surfaces of the uniform cube and sphere placed in the fluid.

3.2 Interaction with a Cube

We place the cube with side length l centered at (x_0, y_0, z_0) in a parabolic velocity profile described by $v(y) = ay^2\hat{x}$. The cube is initially motionless. The following quantities can be analytically computed with symmetry along the z direction:

$$\overleftrightarrow{\tau} = \vec{\nabla}\vec{v} + (\vec{\nabla}\vec{v})^T \quad (6)$$

$$\vec{v} = (v(y), 0) = (ay^2, 0), \quad v_x = ay^2, \quad v_y = 0 \quad (7)$$

$$\vec{\nabla}\vec{v} = \partial_i v_j, \quad (\vec{\nabla}\vec{v})^T = \partial_j v_i \quad (8)$$

$$\overleftrightarrow{\tau} = \begin{pmatrix} \frac{\partial v_x}{\partial x} & \frac{\partial v_x}{\partial y} \\ \frac{\partial v_y}{\partial x} & \frac{\partial v_y}{\partial y} \end{pmatrix} + \begin{pmatrix} \frac{\partial v_x}{\partial x} & \frac{\partial v_x}{\partial y} \\ \frac{\partial v_y}{\partial x} & \frac{\partial v_y}{\partial y} \end{pmatrix}^T = \begin{pmatrix} \frac{\partial v_x}{\partial x} & \frac{\partial v_x}{\partial y} \\ \frac{\partial v_y}{\partial x} & \frac{\partial v_y}{\partial y} \end{pmatrix} + \begin{pmatrix} \frac{\partial v_x}{\partial x} & \frac{\partial v_y}{\partial x} \\ \frac{\partial v_x}{\partial y} & \frac{\partial v_y}{\partial y} \end{pmatrix} \quad (9)$$

$$= \begin{pmatrix} 2\frac{\partial v_x}{\partial x} & \frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \\ \frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} & 2\frac{\partial v_y}{\partial y} \end{pmatrix} \\ = \begin{pmatrix} 0 & 2ay \\ 2ay & 0 \end{pmatrix} \quad (10)$$

$$\overleftrightarrow{\sigma} = -p \overleftrightarrow{I} + \mu \overleftrightarrow{\tau} = \mu \begin{pmatrix} 0 & 2ay \\ 2ay & 0 \end{pmatrix} \quad (11)$$

We assume the pressure is uniform in the x direction, so its effect on the stress tensor can be neglected initially. Using the stress tensor, the force acting on the cube can be found

$$\vec{F}_{net} = -\oint \vec{\sigma} \cdot \hat{n} dA \quad (12)$$

$$\hat{n}_{top} = \hat{y} = (0, 1)^T = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\hat{n}_{bottom} = -\hat{y} = (0, -1)^T = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$$

$$\begin{aligned} \vec{F}_{net} &= -\mu \begin{pmatrix} 0 & 2ay \\ 2ay & 0 \end{pmatrix}_{top} \cdot (0, 1)^T \cdot A_{top} - \mu \begin{pmatrix} 0 & 2ay \\ 2ay & 0 \end{pmatrix}_{bottom} \cdot (0, -1)^T \cdot A_{bottom} \\ &= \mu \begin{pmatrix} 0 & 2a(y_b - y_t) \\ 2a(y_b - y_t) & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot A \\ &= \mu \begin{pmatrix} 2a(y_b - y_t) \\ 0 \end{pmatrix} A \end{aligned} \quad (13)$$

where y_t is the y -value at the top, y_b is the y -value at the bottom, and $A = l^2$ is the surface area of a side of the cube. Therefore, this results in a net force in the x direction acting on the cube equal to

$$2a\mu(y_b - y_t)A = 2a\mu l^3 \quad (14)$$

3.3 Interaction with a Sphere

Next, we place a sphere with radius r_0 centered at (x_0, y_0, z_0) in a parabolic velocity profile described by $v(y) = ay^2\hat{x}$. The sphere is initially motionless. We end up with the same stress tensor locally in the fluid:

$$\vec{\tau} = \begin{pmatrix} 0 & 2ay & 0 \\ 2ay & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (15)$$

The force on the sphere is computed under a spherical coordinate system with the origin at

the center of the sphere:

$$\hat{n} = \frac{\vec{r}}{r} = \frac{(x - x_0, y - y_0, z - z_0)}{r} \quad (16)$$

$$\tau \cdot \hat{n} = \frac{1}{r} \begin{pmatrix} 2ay(y - y_0) \\ 2ay(x - x_0) \\ 0 \end{pmatrix} \quad (17)$$

$$\sigma = \mu \tau \quad (18)$$

$$\vec{F} = \oint \sigma \cdot \hat{n} dA = \frac{\mu}{r} \iint \begin{pmatrix} 2ay(y - y_0) \\ 2ay(x - x_0) \\ 0 \end{pmatrix} r^2 \sin \theta d\theta d\phi \quad (19)$$

$$x - x_0 = r \sin \theta \cos \phi, y - y_0 = r \sin \theta \sin \phi \quad (20)$$

$$x = x_0 + r \sin \theta \cos \phi, y = y_0 + r \sin \theta \sin \phi \quad (21)$$

$$F_x = 2\mu ar \int_0^\pi \int_0^{2\pi} (y_0 + r \sin \theta \sin \phi) r \sin \theta \sin \phi \sin \theta d\theta d\phi = \frac{8\mu}{3} \pi r^3 a \quad (22)$$

$$F_y = 2\mu ar \int_0^\pi \int_0^{2\pi} (y_0 + r \sin \theta \sin \phi) r \sin \theta \cos \phi \sin \theta d\theta d\phi = 0 \quad (23)$$

As expected, the velocity gradient creates a net force in the x direction because the velocity profile is parabolic. The net force is independent of the y position of the sphere in the fluid.

3.4 Numerical Simulation

A mesh is used to discretize the computational domain in the fluid surrounding the cube and the sphere. In the case of the cube, the discretization is straightforward and a rectilinear mesh is used. We obtain almost identical answers between the theoretical approach in equation (14) and the numerical computation.

For the sphere, meshing between a rectilinear mesh and the spherical geometry is more challenging. Determination of the boundary cells intersecting the sphere is done by checking the center position of the cell. If the center position is inside of the sphere, the mesh cell is considered an inside cell, thus it won't contribute to the force and torque calculation; if the center position is outside of the sphere but the center to center distance is less than $R + \frac{\sqrt{3}}{2}\Delta x$ (where Δx is the size of the mesh cell), the mesh cell is marked a boundary cell that will contribute to the force and torque calculation; finally, cells whose centers are more than $R + \frac{\sqrt{3}}{2}\Delta x$ away from the center of the sphere are considered away cells that won't interact directly

with the sphere, thus they won't contribute to the force and torque calculation. An improved but more computationally-demanding method is to iterate through the distances between the center of the sphere and the vertices and midpoints of the sides of the mesh cells. A cell is considered a boundary cell if the minimum distance is equal to or less than the radius of the sphere and the center to center distance is greater than the radius of the sphere.

A challenge the numerical algorithm runs into is the differential area used in the summation algorithm. The cells intersecting with the sphere resulting in irregular areas to be used in the summation.

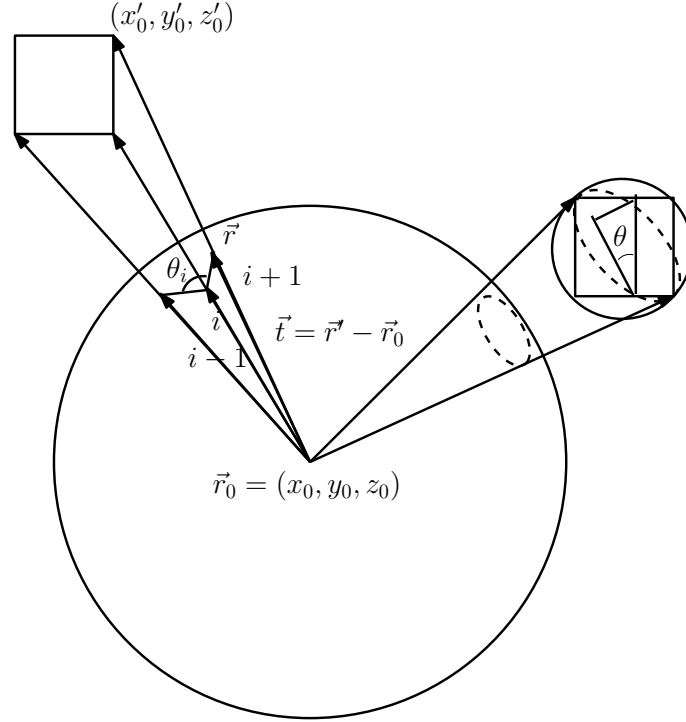


Figure 1: The intersecting area between a small cube and a sphere. Two different approaches are drawn in the diagram. On the left, intersection points between the sphere and the projections of the vertices of the cube are calculated and the intersecting area is computed from the spherical polygon formed by the intersection points. On the right, a circumscribed sphere is used surrounding the cube, then the intersecting area is calculated from the projected area of the square.

There is no available fast algorithm from literature to find the intersection area between a small cube and a sphere. We propose and test two different approaches in this work. The straightforward approach is to project the area of a square to the surface of the sphere to approximate the intersecting area.

$$A_{intersection} = r_0^2 \cdot \frac{dx^2}{(\vec{r}_{c,cube} - \vec{r}_0)^2} \cdot \cos \theta \quad (24)$$

$$\cos \theta = \sqrt{\hat{n}_x^2 + \hat{n}_y^2} \quad (25)$$

where r is the distance from point (x, y, z) to the center of the sphere (x_0, y_0, z_0) , $\vec{r}_{c, cube}$ is the position of the center of the cube, dx is the side length of the rectangular grid cell, θ is the angle between the displacement vector of the center of the cell and the xy plane. This algorithm is relatively fast.

In the 2nd approach, we calculate the intersection points on the surface of the sphere and then use the area of the resulting spherical polygon from equation (30) to approximate the intersection area between the rectangular cells and the sphere based on Figure 1.

$$\beta = \frac{r_0}{\sqrt{(x' - x_0)^2 + (y' - y_0)^2 + (z' - z_0)^2}} \quad (26)$$

$$x = x_0 + \beta(x' - x_0) \quad (27)$$

$$y = y_0 + \beta(y' - y_0) \quad (28)$$

$$z = z_0 + \beta(z' - z_0) \quad (29)$$

$$A = r^2 \left(\sum_{i=1}^n \theta_i - (n-2)\pi \right) \quad (30)$$

$$\theta_i = \arccos \left(\frac{\vec{t}_{i-1} \times \vec{t}_i}{\|\vec{t}_{i-1} \times \vec{t}_i\|} \cdot \frac{\vec{t}_i \times \vec{t}_{i+1}}{\|\vec{t}_i \times \vec{t}_{i+1}\|} \right) \quad (31)$$

$$\vec{t}_i = \vec{r}_i - \vec{r}_{i-1} \quad (32)$$

where (x', y', z') is the position of a vertex of the rectangular cell, $\vec{r}_0 = (x_0, y_0, z_0)$ is the position of the center of the sphere, $\vec{r} = (x, y, z)$ is the position of the intersection point on the sphere by connecting the center of the sphere and the vertex, r_0 is the radius of the sphere, β is the ratio to determine the position of the intersection point on the sphere, A is the area of the spherical polygon, and θ_i is the enclosed angle between neighboring sides of the polygon (see Figure 1) calculated from the tangent directions $\vec{t}_i$ of the polygon edge. The tangent direction itself is calculated from the positions $\vec{r}_i, \vec{r}_{i-1}$ of neighboring vertices of the spherical polygon. This formulation can be generalized more readily to particles of other shapes based on the Gauss-Bonnet theorem.

We populate the velocity profile in an N^3 -resolution rectilinear grid, where $N = 100, 200, \dots$. The sphere representing a particle in fluid is placed in the computational domain. The numerical results confirm the position of the ball placed in the domain has negligible effect on the calculated F_x from equation (22) since the force is position independent in a parabolic velocity

profile. In order to work with a high resolution grid setup, e.g. 1000^3 is a billion grid cells, we developed a compacting algorithm to keep track of the cells intersecting the sphere because the surface stress and force calculation only occurs at these intersecting cells. This significantly reduces memory and computational cost of the algorithm.

The following results (Figure 2) are obtained at various radii of the sphere and grid resolution comparing the analytical force F_x from equation (22) and numerically calculated F_x using the grid. The results show good agreement between the exact analytical and numerically calculated F_x . The calculated F_x is not resolution dependent, thus validating the algorithm.

4 Results

To gain a better understanding of the particle fluid interaction in laminar flow, we formulate a set of equations that govern the fluid flow and the motion of the particle. The particle interacts with the fluid through forces due to pressure and stress. The shear force due to stress also causes rotational motion of the particle. The motion of the fluid and the motion of the particle are coupled.

We explore two simple scenarios to verify the correctness of the method by comparing the results from the analytical derivation and numerical calculation with a parabolic velocity profile. The results from the numerical calculation is in good agreement (at most 5% error) with the analytical derivation. The agreement improves as the grid resolution increases and the particle size increases. The agreement also improves as the radius of the spherical particle increases because the relative resolution of the grid used in numerical calculation increases. For smaller particles, a higher resolution grid is needed. To improve the efficiency of the algorithm at high resolution, a compacting algorithm is used such that only grid cells surrounding the sphere are used to carry out the force and torque calculation.

The correctness of the formulation allows us to generalize the numerical calculation to more realistic velocity profiles, for which an analytical approach is generally not available. Applications of this framework include many natural processes and industrial applications such as microfluidics, air pollution, sediment transport, blood flow, mineral processing, petrochemicals, pharmaceuticals, etc [14] [21] [22] [23] [24]. The proposed approach in this work can provide insights in understanding various phenomena involved in particle-fluid flows.

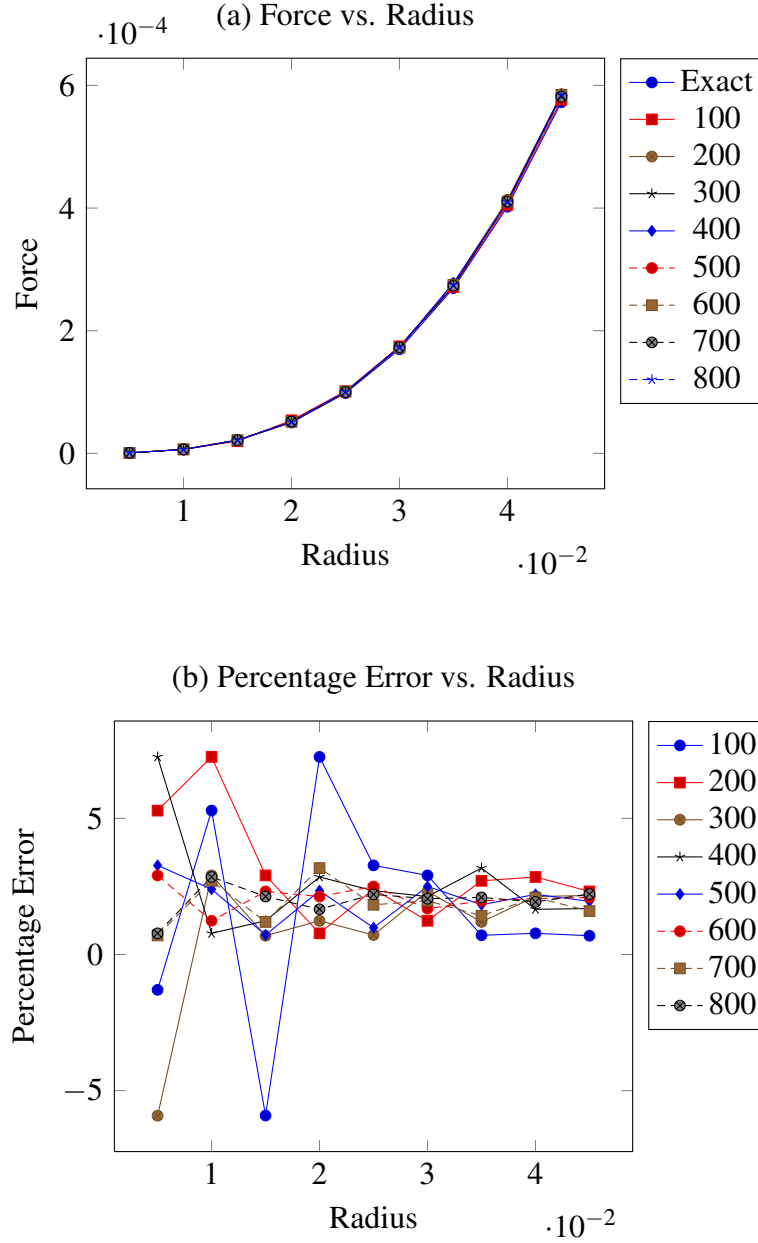


Figure 2: Exact analytical result and numerically calculated force F_x at grid resolutions from 100 to 800 are graphed in (a) and the percentage errors are graphed in (b). The curves in (a) are almost indistinguishable due to the close agreement between the analytical and numerical values. The percentage error graph amplifies the difference at the various rectangular grid resolution used. Higher resolution results show less variability compared with low resolution results.

4.1 Applications in Microfluidics

Inertial focusing occurs in microfluidic systems when particles suspended in a fluid are subjected to a high-speed flow in a microchannel, causing them to align and concentrate at specific locations within the channel. This phenomenon has been extensively studied and has found numerous applications in various fields, particularly in the biomedical domain. The essence

of its applications lies in its ability to differentiate between particles based on size, density, or other characteristics. New techniques based upon inertial focusing are divided into four main groups: sheathless alignment, particle separation, volume reduction, and fluid exchange [14]. In particular, particle separation techniques may benefit from a deeper understanding of the fluid-particle interactions.

Particle separation employs the high-speed flow of particles or cells within a microchannel to separate them into distinct annuli based on size, shape, deformability, or other characteristics. This allows for their separation without the need for additional mechanisms like filters or external fields.

Particle separation has been applied to isolate circulating tumor cells (CTCs) from blood, enabling early cancer detection, monitoring disease progression, and tailoring personalized treatment strategies. While traditional techniques rely on invasive surgeries for tissue acquisition, the collection of CTCs through microfluidics offers a noninvasive alternative known as *Liquid Biopsy*. In diagnostics, particle separation techniques are crucial for concentrating disease-specific biomarkers, enhancing the sensitivity of tests for infectious diseases and cancer. These techniques also support drug discovery and development, enabling the screening of potential therapeutics and the investigation of drug mechanisms [25].

4.2 Improvements and Future Work

There are a few future improvements. First, an adaptive grid can be used such that low resolution grids can be used in regions of the fluid where particle-fluid interaction is unnecessary. Second, turbulent processes can be included in the formulation to model particle-fluid interaction in the turbulence regime. Third, the discrete force and torque calculation on the surface of a sphere can be further refined and improved to address the geometry difficulty involved between rectilinear cells and the spherical surface. Finally, the algorithm can be parallelized such that greater computing power can be harnessed to perform particle-fluid interactions when a large number of particles exist in the fluid flow.

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